

3-Methyl-1-nitrobutane
627-67-8 | DTXSID90211769

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 7.91 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.71e-01

Confidence level: 7.91e-01

Nearest Neighbors from the Training Set

Image not found

Ethyl methyl sulfide

Measured: 6.88

Predicted: 121

Image not found

Ethyl 2-bromoisobutyrate

Measured: 7.79

Predicted: 3.11

Image not found

Ether, isobutyl methyl

Measured: 3.79

Predicted: 201

Image not found

2,3-Dimethylbutan-2-ol

Measured: 12.0

Predicted: 5.17

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Propane, 2-methyl-2-nitro-

Measured: 16.9

Predicted: 9.73